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Theoretical Study of Iron Filled Carbon Nanotubes MARIANA WEISSMANN, C.N.E.A., Buenos Aires, Argentina, GRISELDA GARCIA, MIGUEL KIWI, RICARDO RAMIREZ, Facultad de Fisica, PUC, Chile, CHU-CHUN FU, CEA, Saclay, France — We have investigated, using ab-initio methods, the geometry and magnetic structure of free standing and encapsulated iron nanowires, both in perfect and defective single wall carbon nanotubes. The geometries adopted consist of two layers of iron atoms per unit cell, arranged in hcp(0001) and bcc(011) structures, repeated periodically along the wire axis, When the ratio of the nanowire to nanotube diameter is small there is an attractive interaction among them and the density of states at the Fermi energy corresponds to a single spin orientation, as for the free standing nanowires. These systems are therefore potentially interesting for spintronics. When the same ratio is close to one the systems are less stable and a tendency towards antiferromagnetic ordering is observed due to the confinement.

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